PRECISE SEMI-EXPERIMENTAL EQUILIBRIUM STRUCTURE OF THIAZOLE (C_3H_3NS)

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Thiazole (C_3H_3NS, C_s, μ_a = 1.286 D, μ_b = 0.966 D) is a five-membered aromatic heterocycle containing a 1,3-substituted sulfur and nitrogen. We analyzed the rotational spectra of thiazole and twenty-one of its isotopologues from 130 – 360 GHz. Heavy atom ^{13}C, ^{34}S, ^{33}S, and ^{15}N isotopologues were observable in the rotational spectrum of the normal isotopologue at their natural abundance. Two syntheses were performed to generate a variety of deuterium-substituted isotopologues, resulting in multiple isotopic substitutions of each atom in the molecule. The resultant determinable rotational constants were computationally corrected for vibration-rotation interactions and electron mass with CCSD(T) calculations and 22 total isotopologues were least-squares fit to afford the semi-experimental equilibrium structure (r_e^{SE}). Theoretical structures were computed at several levels of theory up to CCSD(T)/cc-pCV5Z. The quintuple zeta structure was further refined to account for extrapolation to the complete basis set limit, residual electron correlation beyond CCSD(T), relativistic effects, and the diagonal Born-Oppenheimer correction. The resultant r_e^{SE} structure and best theoretical structure are compared.